

## ENERGY TRANSFER DYNAMICS IN VIBRATIONAL POLARITONS: A QUASI-CLASSICAL APPROACH

Patricia Adeoye, and Dmitri Kilin

*Department of Chemistry and Biochemistry, North Dakota State University, Fargo, ND 58102*

The study of vibrational polaritons has received attention in the Chemistry community not only because of their influence on chemical reactions but also because the hybrid characteristic of vibrational polaritons makes them suitable to possess interesting properties from both molecular and photonic systems and this can lead to new properties that are useful in photonic and quantum technology.<sup>1</sup>

This research investigates vibrational polaritons, the interplay between light and molecular vibrations, employing a quasi-classical treatment of cavity modes. The study focuses on discerning the trajectories of the expectation value of the field amplitude, derived from the Heisenberg equation of motion for the nuclear position of the molecular system and the amplitude of the electric field. This study delves into the concepts of energy transfer between photons (electromagnetic degree of freedom) and phonons (vibrational degree of freedom), unveiling insights into this interaction without perturbing chemical bonds or inducing reactions. The molecular dynamics calculation of the Hydrogen fluoride (H-F) molecule and the examination of the photonic degree of freedom within the realm of vibrational polaritons provide a perspective on the relationship between light and matter. Our approach integrates a quasi-classical approach/approximation, contributing to an understanding of how energy dynamically traverses between light and matter. Notably, the results highlight trends as the coupling strength intensifies. A noticeable decrease in the expectation value of the field signifies strengthened interactions between light and matter. Additionally, the consistent reduction in the period of beat indicates dynamic changes in the oscillatory patterns within the cavity. Building upon our prior exploration of vibrational polaritons fully quantumly, we reveal similarities in the observables derived from these approaches such as a change in equilibrium bond length in the molecule and equilibrium strength of the electric field. Furthermore, our findings illuminate a departure from harmonic oscillations in the cavity as the coupling strength intensifies. This departure is attributed to the large amplitudes of the field, resulting in a less harmonic oscillation profile. This observation provides insights into the effects of increased coupling strength on energy states, culminating in the attainment of maximum energy within the systems. The identified trends in interaction strength, oscillatory behaviour, and energy states pave the way for future studies aimed at manipulating light-matter interactions within materials. This work holds significant promise for applications in quantum optics, materials science, and energy transfer research.

(1) Xiong, W. Molecular Vibrational Polariton Dynamics: What Can Polaritons Do? *Accounts of Chemical Research* **2023**, 56 (7), 776-786. DOI: 10.1021/acs.accounts.2c00796.